

Description of Additional Supplementary Files

File name- Supplementary Movie 1

File description- The total electron density: This movie shows the time-dependent evolution of the OCS electron density projected on the xy-plane during the interaction with a 7 fs laser pulse at 800 nm having a peak intensity of 3.2 PW cm^{-2} . In this movie, the initial bend angle of OCS is 172 degrees and the laser polarization angle relative to the x-axis is 40 degrees. The solid black lines show the trajectory of ions in time. The grey gridlines indicate $x = y = 0$.

File name- Supplementary Movie 2

File description- The total electron density: This movie shows the dynamics of the OCS electron density projected on the xy-plane under the interaction of a 7 fs laser pulse at 800 nm having a peak intensity of 2.8 PW cm^{-2} . In this movie, the initial bend angle of OCS is considered as 172 degrees and the laser polarization angle relative to the x-axis is assumed to be 0 degrees. The solid black lines show the trajectory of ions in time. The grey gridlines indicate $x = y = 0$.

File name- Supplementary Movie 3

File description- Orbital movie (HOMO): This movie displays the time-dependent evolution of the highest occupied molecular orbital (HOMO) in the OCS molecule (π orbital) projected on the xy-plane during and after its interaction with a 7 fs laser pulse at 800 nm having a peak intensity of 3.2 PW cm^{-2} . During the laser-molecule interaction, one can see a charge transfer phenomenon within the OCS molecule particularly when the laser field reaches its peak intensity. Remarkably, we observe charges departing from the molecule at the angle of 40/140 degrees (along the laser polarization direction) during these peak moments. Furthermore, the movie illustrates the intriguing transformation of the π orbital into three separate atomic p orbitals as the OCS molecule dissociates into its constituent ions. This visual representation offers a vivid depiction of the complex ultrafast dynamics captured in our study, providing valuable insights into laser-induced ionization and the molecular dissociation processes.

File name- Supplementary Movie 4

File description- Orbital movie (HOMO-1): This movie presents the time-dependent evolution of the HOMO-1 in the OCS molecule (σ orbital) projected on the xy-plane. The laser parameters are the same as Supplementary Movie 3. Here, the transformation of the σ orbital into two p-orbitals (distributed around sulfur and oxygen) and one s-orbital (distributed around carbon) is observed.

File name- Supplementary Movie 5

File description- Orbital movie (HOMO-2): In this movie, the time-dependent evolution of the HOMO-2 in the OCS molecule (π orbital) projected on the xz-plane is observed. The laser parameters are the same as Supplementary Movie 3. As can be seen, the π orbital transforms into three p-orbitals.